

LA-UR-16-27839

Approved for public release; distribution is unlimited.

Title: NJOY and MCNP

Author(s): Conlin, Jeremy Lloyd

Intended for: NJOY class

Issued: 2016-10-12

Disclaimer:

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

NJOY and MCNP



Jeremy Lloyd Conlin

October 26, 2016
LA-UR-16-XXXXX



Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA

Using New Data

- **Updated ^{238}U from ENDF/B-VIII.0**
 - How does this affect your calculation?
- **Exercise:**
 - Process ENDF/B-VIII.0 evaluation for ^{238}U into an ACE file.
 - 92u238 directory contains evaluation file
 - Start with NJOY input deck for ^{235}U

Solution

- Replace all instances of ^{235}U material number (9228) with ^{238}U material number (9237)

```
moder
1 -21/                                card1
'moder iopt=1, extract mat 9237 from input tape'/card2
20 9237/                                card3
0/                                      repeat card3, 0=moder is done
reconr
-21 -22/                                card1
'reconr/pendf tape for mat 9237'/      card2
9237 7/                                card3
.001/                                    card4
...
0 /                                      repeat card3, 0=reconr is
broadr
-21 -22 -23/                            card1
9237 1 0 0/                            card2
.001 -2E4/                              card3
293.6                                    card4
0/                                      repeat card2, 0=broadr is done
```

Using One-Off Data in MCNP

- **Rename/move ACE file**

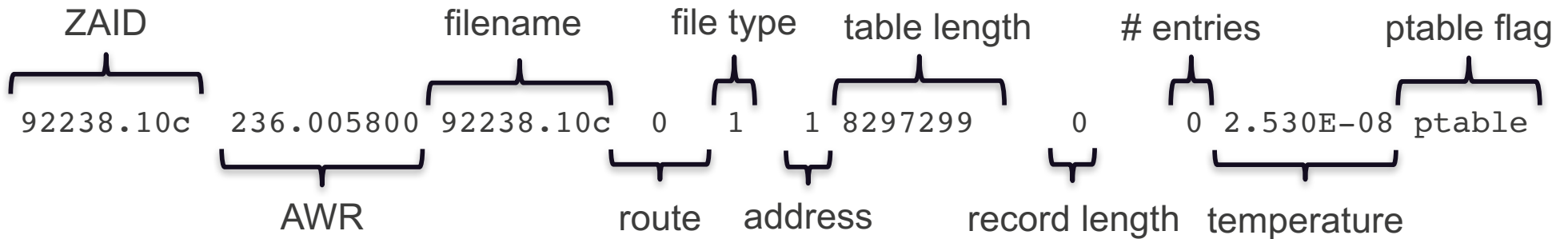
- tape34 in this exercise
- Place file (92238.10c) in same directory as MCNP input deck

- **Use the xSn card in MCNP**

- n 1 to 999
- The entries for the xSn card are identical to those in XSDIR (tape35 in this exercise)

| | | | | | | | | | | |
|-----------|------------|-----------|---|---|---|---------|---|---|-----------|--------|
| 92238.10c | 236.005800 | 92238.10c | 0 | 1 | 1 | 8297299 | 0 | 0 | 2.530E-08 | ptable |
|-----------|------------|-----------|---|---|---|---------|---|---|-----------|--------|

XSDIR Entry



1. ZOID
2. Atomic Weight Ratio
3. Filename of ACE file
4. "Route" to ACE file (zero if no path)
5. File Type (1 or 2, ascii or binary)
6. Address—on what line does the data begin
7. Table length—How many numbers in table
8. Record length (unused for Type 1)
9. Number of entries per record (unused for Type 1)
10. Temperature (MeV)
11. Probability Table flag—whether or not there are probability tables

Comparing k_{eff} results

| | ENDF/B-VII.1 | ENDF/B-VIII.0 |
|-------|--------------|---------------|
| Big10 | 1.00432 (33) | 1.01269 (37) |



What
Happened!?!

Doppler Broadening Energy Limits

- **From the NJOY manual:**

```
! thnmax A possible upper limit for broadening and thinning.  
! The actual upper limit is the lowest of (i) this input  
! value; (ii) the end of the resolved resonance range;  
! (iii) the lowest reaction threshold; or (iv) 1.0 MeV.  
!  
! A negative value for thnmax forces the Doppler  
! broadening upper limit to be abs(thnmax) irrespective  
! of the other conditions.
```

- **End of resolved resonance range:**

- 20 keV

- **Lowest threshold reaction:**

- ~40 keV in ENDF/B-VII.1

- ~0.1 keV in ENDF/B-VIII.0

How to find End of Resolved Resonance Range

- Save RECONR results in ascii format

```
reconr
-21 -22/
'reconr/pendf tape for mat 9237'/
9237 7/
.001/
'the following reaction types may be added'/
'    mt152    bondarenko unresolved'/
...
0 /
-- Save output from RECONR
moder
-22 52/

card1
card2
card3
card4
card5 (repeat 7 times)

repeat card3, 0=reconr is done

/card1
```

How to find End of Resolved Resonance Range

- Look at MF=2, MT=151 in output

| | | | | | | | | | |
|------------|------------|---|---|---|--|-------|------|--------|---|
| | | | | | | 9237 | 0 | 0 | 0 |
| 9.223800+4 | 2.360058+2 | 0 | 0 | 1 | | 09237 | 2151 | | 1 |
| 9.223800+4 | 1.000000+0 | 0 | 0 | 1 | | 09237 | 2151 | | 2 |
| 1.000000-5 | 2.000000+4 | 0 | 0 | 0 | | 09237 | 2151 | | 3 |
| 0.000000+0 | 9.433790-1 | 0 | 0 | 0 | | 09237 | 2151 | | 4 |
| | | | | | | 9237 | 2 | 099999 | |

Begin of
RRR

End of
RRR

Exercise

- **Modify your NJOY input deck to Doppler broaden to correct limit**

Solution

```
broadr
```

```
-21 -22 -23/
```

```
9237 1 0 0/
```

```
.001 -2E4/
```

```
293.6
```

```
0/
```

```
card1
```

```
card2
```

```
card3
```

```
card4
```

```
repeat card2, 0=broadr is done
```

Comparing k_{eff} results

| | ENDF/B-VII.1 | ENDF/B-VIII.0 | ENDF/B-VIII.0-2 |
|-------|--------------|---------------|-----------------|
| Big10 | 1.00432 (33) | 1.01269 (37) | 1.00599 (36) |

That's better

Adding Data to MCNP's Data

- **Move ACE files some place under DATAPATH directory**
 - Place inside a directory (myACEFiles)
 - Add entry to XSDIR

```
92238.10c 236.005800 myACEFiles/92238.10c 0 1 1 8297299 0 0 2.530E-08 ptable
```

- **XSDIR directory order is important**
 - MCNP searches from the top until it finds a matching ZAID

```
directory
1001.90c 0.999167 endf71x/H/1001.720nc 0 1 4 8177 0 0 2.530100E-08
1001.91c 0.999167 endf71x/H/1001.721nc 0 1 4 8177 0 0 5.170400E-08
...
sio2.10t 27.737000 ENDF71SaB/sio2.10t 0 1 1 2010074 0 0 2.530E-08
sio2.11t 27.737000 ENDF71SaB/sio2.11t 0 1 1 1968401 0 0 3.016E-08
...
1001.80c 0.999167 endf71x/H/1001.710nc 0 1 4 17969 0 0 2.530100E-08
1001.81c 0.999167 endf71x/H/1001.711nc 0 1 4 17969 0 0 5.170400E-08
1001.82c 0.999167 endf71x/H/1001.712nc 0 1 4 17969 0 0 7.755600E-08
```